ENTROPY IN BIOLOGY

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Lecture 3 — appendix

Uniqueness & positivity of the steady state of a finite continuous-time Markov chain under the assumption that any state can be reached from any other state by a sequence of allowed transitions.

Note: This is usually proved by considering the embedded discrete-time Markov chain, but here we stay within the continuous-time framework.

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Steady state of a finite continuous-time Markov chain

We consider a continuous-time Markov chain with n states indexed by $1 \cdots n$

Let r_{ij} be the probability per unit time of a transition $i \to j$ when the system is in state i. Then

(1) $$r_{ij} \geq 0$$

We assume, moreover, that it is possible to get from any state to any other state by means of a sequence of allowed transitions. This means that for any pair (i,j) with $i \neq j$, there exists a sequence of states

(2) $$k_0 \cdots k_s$$

such that $i = k_0$, $j = k_s$, and

(3) $$r_{k_{l-1}, k_l} > 0 \quad \text{for } l = 1 \cdots s$$

Let p_i be the steady-state probability that the system is in state i. Then

(4) $$\sum_{i=1}^{n} \left(p_i r_{ij} - p_j r_{ji} \right) = 0, \quad j = 1 \cdots n$$

and

(5) $$\sum_{i=1}^{n} p_i = 1$$

We claim that there exists a unique $p = (p_1 \cdots p_n)$ satisfying (4-5), and also that $p_i > 0$ for $i = 1 \cdots n$.

To prove this, we start by putting (4) in matrix form.

Let the $n \times n$ matrix R be defined by

(6) $$R_{ij} = r_{ij} \quad , \quad i \neq j$$

(7) $$R_{jj} = -\sum_{\substack{i=1 \\ i \neq j}}^{n} r_{ij} \quad , \quad j = 1 \cdots n$$

Then (4) is equivalent to

(8) $$pR = 0$$

Remark: If there ~~were~~ are any nonzero diagonal elements of r, they cancel out of (4) and therefore have no effect on p. Consistent with this, they are discarded in the construction of R.

For future reference, it will be useful to interchange the indices i and j in (7). This gives

(9) $$R_{ii} = -\sum_{\substack{j=1 \\ j \neq i}}^{n} r_{ij} = -\sum_{\substack{j=1 \\ j \neq i}}^{n} R_{ij} \quad , i=1 \cdots n$$

and of course this can also be written as

(10) $$\sum_{j=1}^{n} R_{ij} = 0 \quad , \quad i = 1 \cdots n$$

Because of (10), the rank of R is at most $(n-1)$, and we claim that it is equal to $(n-1)$. To show this, we consider ~~that~~ the equation

(11) $$Rx = 0$$

which can be written as

(12) $$\sum_{\substack{j=1 \\ j\neq i}}^{n} R_{ij}(x_j - x_i) = 0, \quad i = 1 \cdots n$$

Now let

(13) $$x_* = \min_{1 \le i \le n} x_i$$

(14) $$I_* = \{ i : x_i = x_* \}$$

Since the set $\{1 \cdots n\}$ is finite, it is obvious that x_* exists and that I_* is not empty.

We claim that

(15) $$I_* = \{1 \dots n\}$$

If not, since I_* is not empty, we can choose a pair of states (i, j) such that

(16) $$i \in I_* \text{ and } j \notin I_*$$

By hypothesis there is a walk as described by (2-3) from i to j, and along this walk there must be at least one step from i' to j' such that

(17) $$i' \in I_* \text{ and } j' \notin I_*$$

For this step (as for every step along the walk), we have

(18) $$R_{i'j'} > 0$$

Now consider equation (12) in the special case $i = i'$. Since $i' \in I_*$, it reads

(19) $$\sum_{\substack{j=1 \\ j \neq i'}}^{n} R_{i'j} \left(x_j - x_* \right) = 0$$

Since every term on the left-hand side of (19) is non-negative, every term must separately be equal to zero. In particular

(20) $$R_{i'j'} \left(x_{j'} - x_* \right) = 0$$

and since $R_{i'j'} > 0$, this implies that

(21) $$x_{j'} = x_*$$

contrary to the statement that $j' \notin I_*$.

This contradiction proves that $I_* = \{1 \ldots n\}$, i.e., that

(22) $$x_i = x_* \, , \quad i = 1 \ldots n$$

This shows that the null space of R is at ~~least~~ most one-dimensional, and indeed it is exactly one-dimensional, since it follows immediately from (12) that any x with all components equal satisfies $Rx=0$.

Thus, $\operatorname{rank}(R)=n-1$, as claimed.

Now let p be a nontrivial solution of $pR=0$. Such a p exists, since $\operatorname{rank}(R)=n-1$. Since p is nontrivial, there is at least one value of i, say i_0, such that $p_{i_0} \neq 0$. If $p_{i_0} < 0$, we change the sign of p, and if $p_{i_0} > 0$, we leave p alone. Either way, we end up with a solution of $pR=0$ with at least one positive component. Now let

(23) $$I_+ = \{ i : p_i > 0 \}$$

Then I_+ is non-empty, since $i_0 \in I_+$.

We claim that

(24) $$I_+ = \{1 \cdots n\}$$

If not, then

(25) $$I_+^c = \{i : p_i \leq 0\} \neq \phi$$

In equation (4), sum both sides over $j \in I_+$, and split the sum over i into two parts, $i \in I_+$ and $i \in I_+^c$. The result is

(26) $$\sum_{i \in I_+} \sum_{j \in I_+} (p_i r_{ij} - p_j r_{ji})$$

$$+ \sum_{i \in I_+^c} \sum_{j \in I^+} (p_i r_{ij} - p_j r_{ji}) = 0$$

In this equation, the first double-sum is zero by symmetry. In the second double sum $p_i \leq 0$ and $p_j > 0$, since $i \in I_+^c$ and $j \in I_+$. Thus

every term is non-positive, so every term must be zero.

This gives

(27) $$p_i r_{ij} = p_j r_{ji}$$

for all (i,j) such that

(28) $$i \in I_+^c \quad \text{and} \quad j \in I_+$$

Equation (27) cannot be true, however, if (i,j) satisfies (28) and if $r_{ji} > 0$, since the left-hand side of (27) is then non-positive but the right-hand side is positive. Thus, we have a contradiction if $\exists (i,j)$ satisfying (28) with $r_{ji} > 0$. But there must exist such a pair (i,j) because of the hypothesis that it is possible to get from any node to any other node by a sequence of allowed transitions.

If there is no pair (i,j) satisfying (28) with $r_{ji} > 0$, then it is impossible to get from a node in I_+ to a node in I_+^c. Since the assumption that I_+^c is non-empty leads to a contradiction, we conclude that $I_+^c = \phi$ and therefore that $I_+ = \{1 \ldots n\}$, as claimed. Thus, all of the components of p are positive.

Recall that we started with an arbitrary non-trivial solution of $pR=0$ and that we changed the sign of p if necessary to make one component positive. Thus, the actual conclusion of the foregoing is that any non-trivial solution of $pR=0$ has all of its components positive or all of its components negative (and in particular none of its components are zero).

Now let $\tilde{p}$ be any nontrivial solution of $\tilde{p}R=0$.

As shown above, such a $\tilde{p}$ exists, and has all of its components positive or all of them negative. Since $\mathrm{rank}(R)=n-1$, the most general solution of $pR=0$ is

(29) $$p = \alpha \tilde{p}$$

with any real scalar α. Then p satisfies the normalization condition (5) if and only if

(30) $$\alpha = 1 \Big/ \sum_{j=1}^{n} \tilde{p}_j$$

The denominator in (30) cannot be zero, since all of the components of $\tilde{p}$ are positive or all of them are negative. It follows that the vector p with components

(31) $$p_i = \tilde{p}_i \Big/ \sum_{j=1}^{n} \tilde{p}_j$$

is the unique solution to (4-5), and also that $p_i > 0$ for every $i \in \{1 \cdots n\}$ $\square$